Plasma-material interaction modeling work at the UIUC

J.P. Allain, D.A. Alman,

M. Nieto, M.D. Coventry,

and D.N. Ruzic

University of Illinois, Urbana-Champaign

Department of Nuclear, Plasma and Radiological Engineering

Plasma-Material Interaction Group

ALPS Meeting, Princeton, New Jersey
November 6-8, 2002

Outline of Work at the UIUC

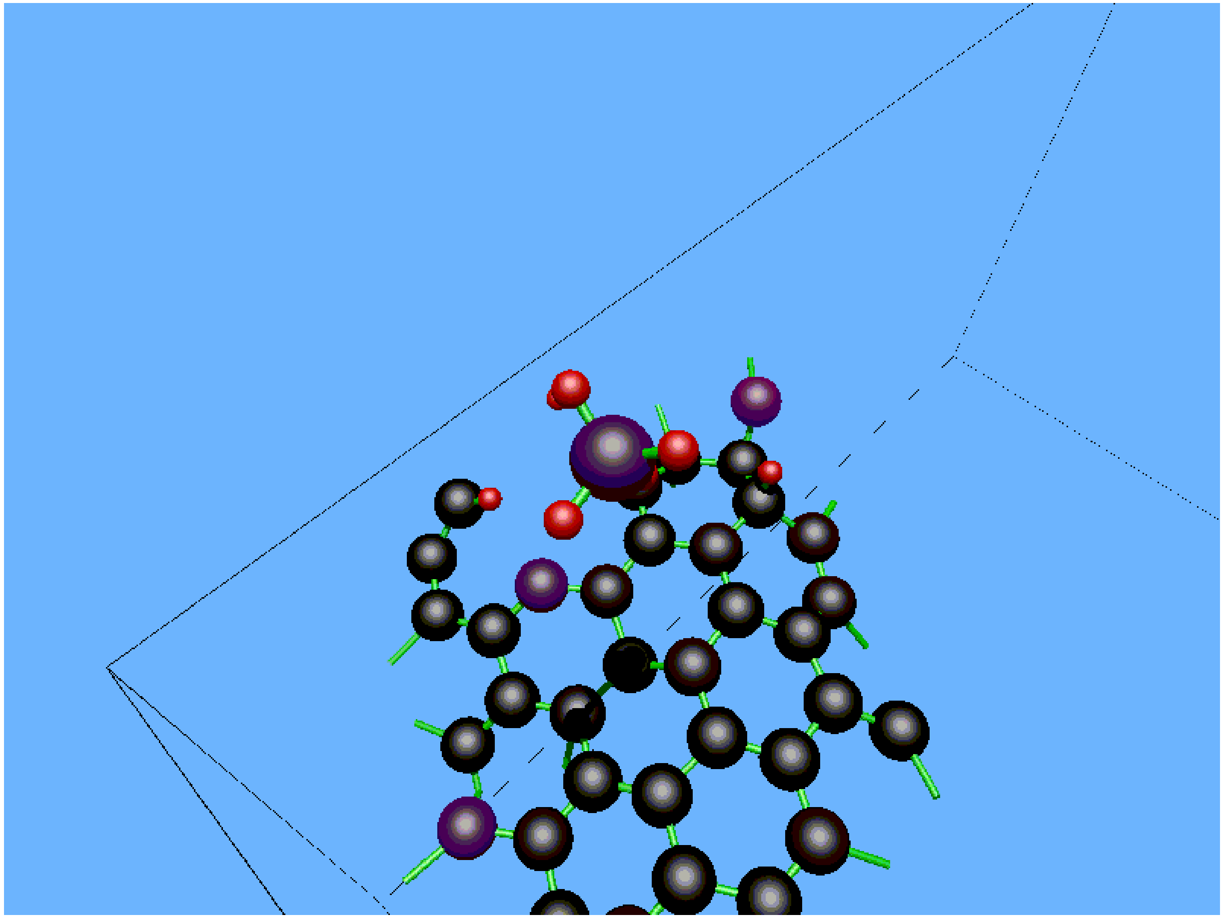
- Molecular Dynamics simulations of hydrocarbon plasma-material interaction
- Molecular Dynamics simulations of liquid lithium to study low energy reflection
- Analytical studies of backscattered and sputtered charge fraction at low energies
- FIRE modeling of plasma-material interactions at the first wall and divertor regions
- Liquid metal erosion work in IIAX

1867 ILLINOIS

Alps

PLASMA MATERIAL INTERACTION GROUP
University of Illinois at Urbana-Champaign

Methane incident at 5 eV and 45 degrees – Breakup

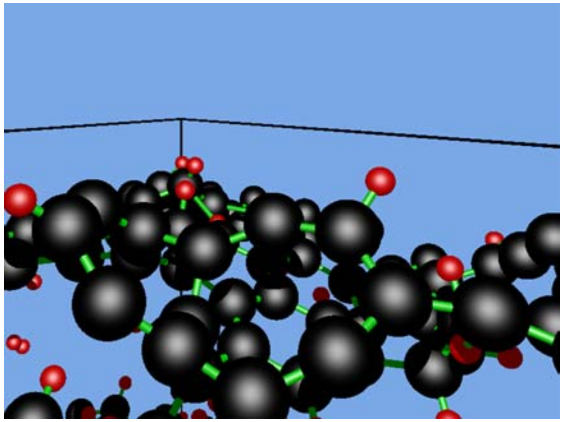


Molecular dynamics modeling of carbon based surfaces

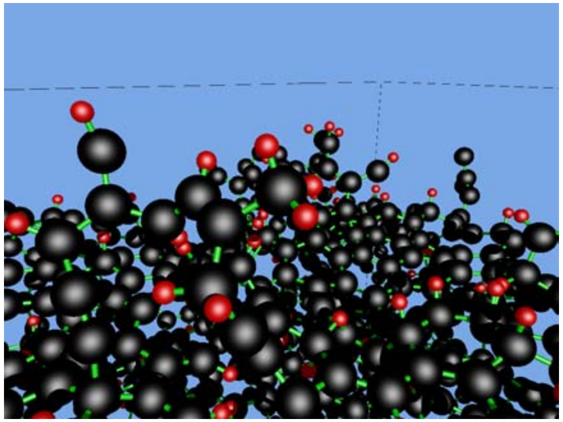
- Determined reflection coefficients for carbon dimers (C_2) and trimers (C_3)
  - Data, together with previous MolDyn results, used in WBC modeling of DiMES hydrocarbon spectroscopy experiment
- Work is ongoing to extend the hydrocarbon potential to higher energies
  - Brenner potential describes the bonding region of the hydrocarbon potential well
  - The small-separation, repulsive portion is not as good - meaning higher energy collisions are less accurate
  - Higher energy capability is needed for above DiMES modeling, for example, where the plasma temperature is 20 eV
  - A new high-energy potential has been implemented for energies above 20 eV using the Kr-C potential splined to the Brenner potential

Carbon-based surfaces used

- Up to now a hydrogen saturated graphite surface has been used
  - Prepared by bombarding originally pure graphite surface with hydrogen
- Developed a "soft" carbon layer
  - Formed by redeposition of thousands of hydrocarbons on an originally pure graphite surface
- In experiments, these layers tend to be:
  - Polymer-like
  - Less dense
  - Higher H:C ratio
  - Weakly bound → larger sputtering yield
- Reflection simulations of hydrocarbons from soft layers in progress
  - Initial results show less reflection



Previous:
H implanted in graphite, result ~0.4 H:C



New:
"soft" layer of redeposited hydrocarbons

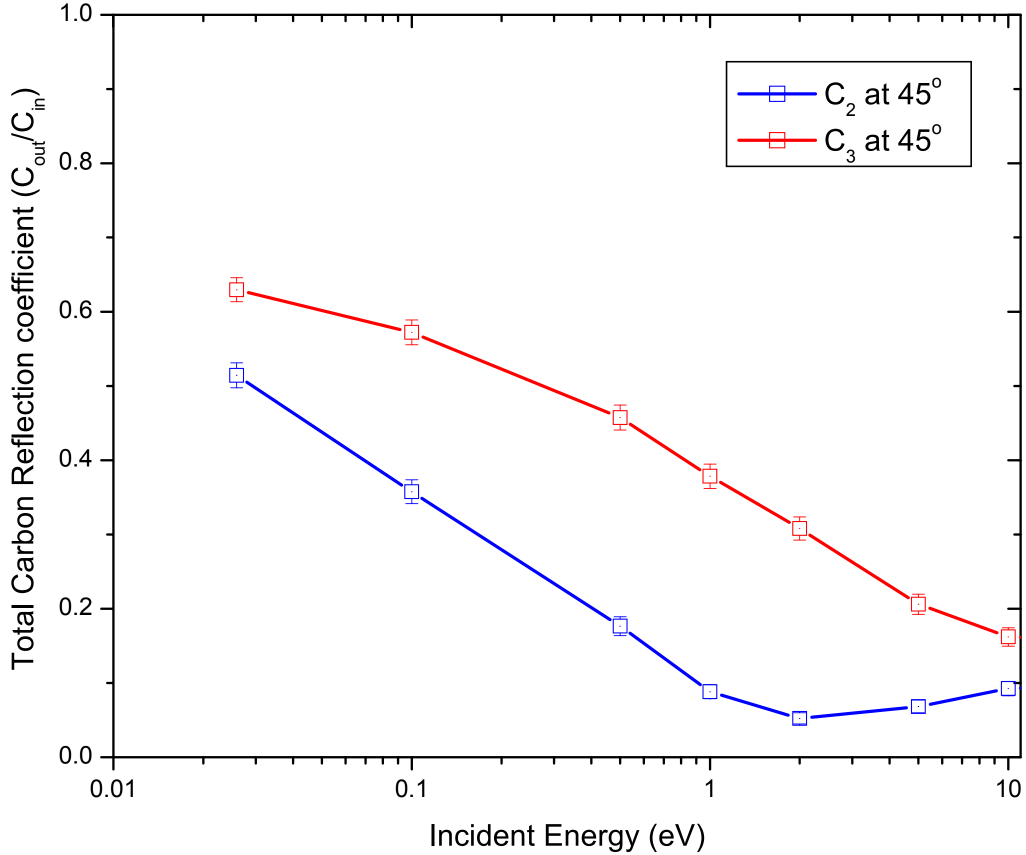
ILLINOIS

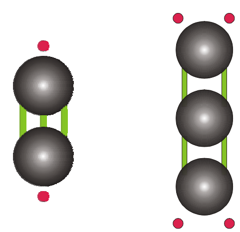
Alps

PLASMA MATERIAL INTERACTION GROUP
University of Illinois at Urbana-Champaign

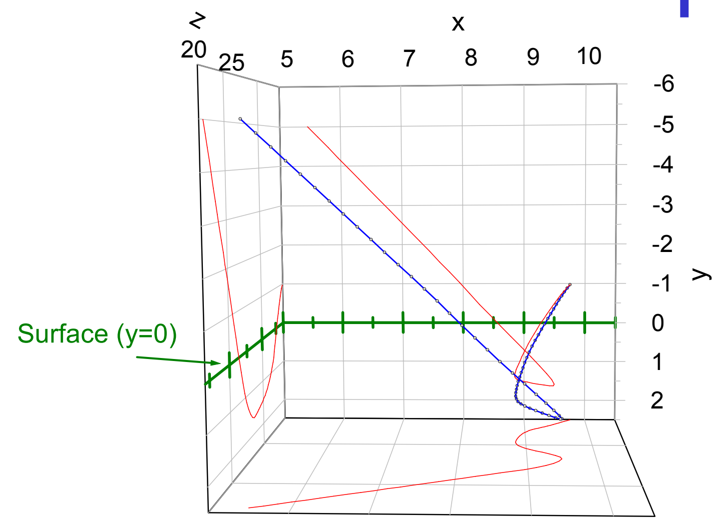
Reflection of Carbon dimer and trimer molecules

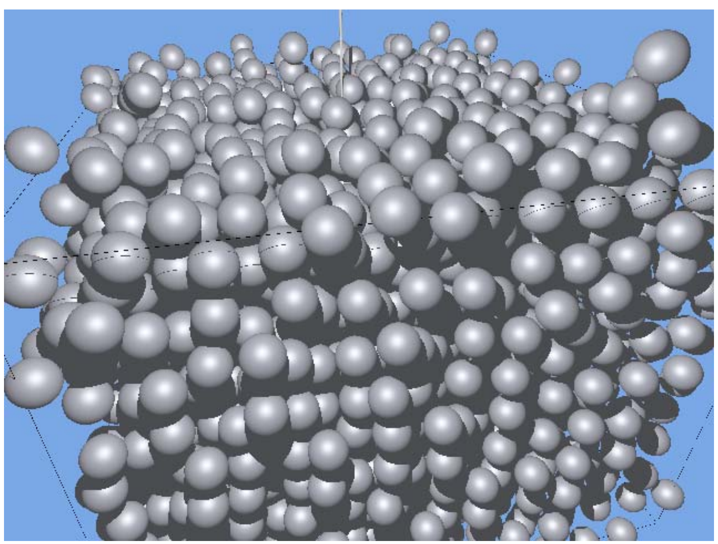
- Carbon dimers tend to stick more readily than trimers
- We're investigating the physics behind this behavior
- The fully bonded central atom in the C_3 molecule my play an important role
  - Repulsive forces between this atom and the surface push the entire molecule away from the surface
  - C_3 then reflects more





MD modeling of lithium bombardment on liquid lithium surfaces

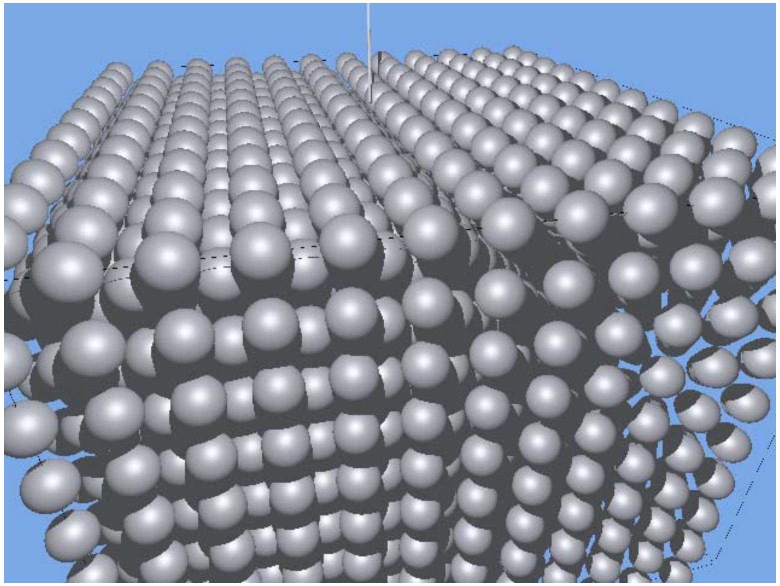


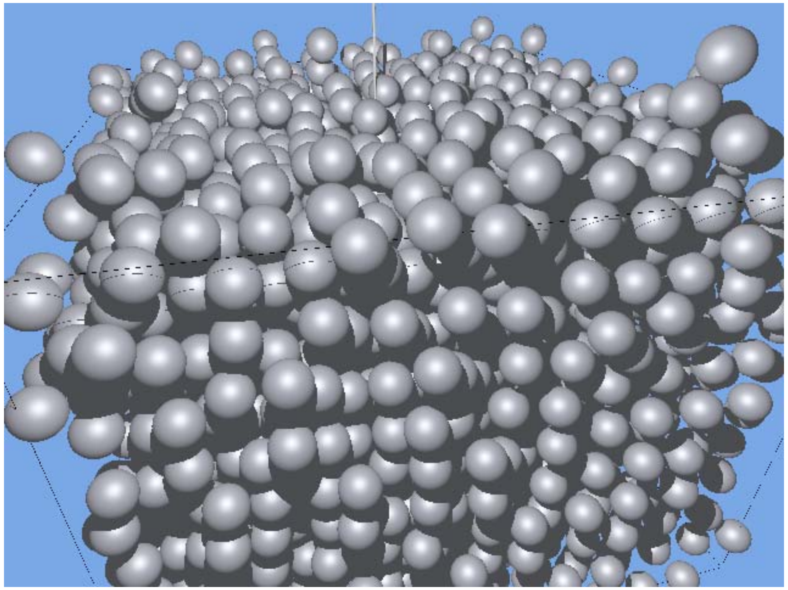


- Investigation of reflection of lithium atoms on liquid lithium surfaces continues
  - 0.35 and 2 eV incident energy
  - 45 degrees incident angle
  - 473 K and 723 K surface temperatures
- Major changes have been made to the code to better incorporate lithium
  - Enabling lithium runs to be integrated into the distributed computing system already in use for hydrocarbon modeling (giving ~10x speed-up)
  - Calculation of ion fraction of reflected/sputtered atoms now built in
  - New liquid lithium potential data included†

†L.E.Gonzalez, private communication (2002).

Liquid lithium simulation setup





- Temperature control is achieved by using a simple velocity scaling technique at each time step[1-3] to maintain the desired temperature at the edges of the surface.
- The resulting target surface is an amorphous liquid lithium surface 42.2 by 42.2 Å and 34.2 Å deep.

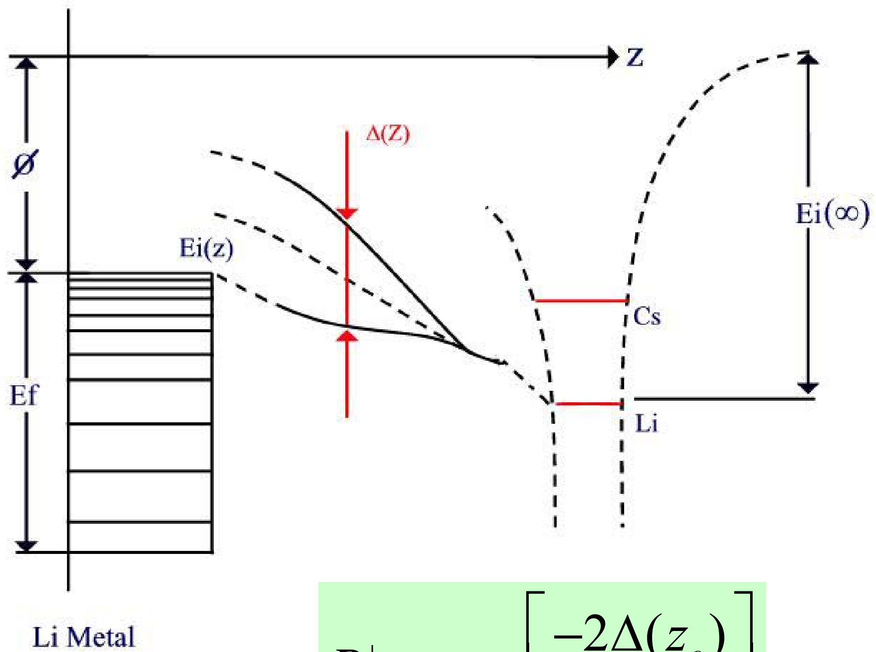
1. L. V. Woodcock, Chem. Phys. Lett. **10**, 257 (1970).
2. D. J. Evans, Mol. Phys. **37**, 1745 (1979).
3. T. Schneider and E. Stoll, Phys. Rev. B **13**, 1216 (1976).

ILLINOIS

Alps

PLASMA MATERIAL INTERACTION GROUP
University of Illinois at Urbana-Champaign

Charge state of lithium reflected particles at low energy



$$P^{+} = \exp\left[\frac{-2\Delta(z_c)}{\hbar \alpha v_p}\right]$$

- Analytical model developed by R. Brako and D.M. Newns[1] for the charge state of backscattered alkali atoms from metals.
- The model assumes that a single spinless atomic orbital participates in the charge transfer and uses the Newns-Anderson Hamiltonian to model the coupling of the atomic state of the particle to that of the metal.
- The model has found success in various areas of surface physics and has been found to accurately predict a number of experimental data including backscattering from alkali metals.

1. R. Brako and D.M. Newns, Rep. Prog. Phys. 52 (1989) 655.
2. J.B. Martson, et. al., Phys. Rev. B 48 (11) (1993) 7809.
3. H. Gnaser, "Low-Energy Ion Irradiation of Solid Surfaces", Springer, Berlin, 1999.
4. M.L. Yu, in "Sputtering by Particle Bombardment III", Springer, Berlin, 1991

Analytical solution in the Newns-Andersen Model

We have the spinless Newns-Andersen Hamiltonian which correlates the states of the outgoing particle state with the electronic state of the surface.

$$H(t)=\sum_{a,i}\left[\varepsilon_a^{(1)}(t)P_1+\varepsilon_a^{(2)}(t)P_2\right]c_a^{\dagger i}c_{ai}+\sum_{k,i}\varepsilon_k c_k^{\dagger i}c_{ki}+\left(\frac{1}{N}\right)^{1/2}\sum_{a,k,i}\left(\left[V_{a;k}^{(1)}(t)P_1+V_{a;k}^{(2)}(t)P_2\right]c_a^{\dagger i}c_{ki}+H.c.\right)$$

The tunneling probability is determined by the magnitude of the transition matrix element, V_{ak} between the atomic state $|a\rangle$ and the metal state $|k\rangle$. The atomic level is broadened in energy and the resonance level is a function of the distance from the surface[1], *z*. To calculate the ionization probability, P^+ one needs to know how Δ and $\varepsilon_a(z)$ vary along the outgoing particle trajectory, these can be approximated by[2]:

$$\varepsilon_a(z)=-I+\frac{e^2}{4(z-z_{im})}+V_{\max}$$

obtain z_c

$$\Delta(z)=\Delta_o\exp(-\alpha z)$$

1. P. Nolander and J.C. Tully, Phys. Rev. B 42 (9) (1990) 5564.
2. N.D. Lang, Phys. Rev. B 27 (4) (1983) 2019.

Analytical solution in the Newns-Andersen Model (cont.)

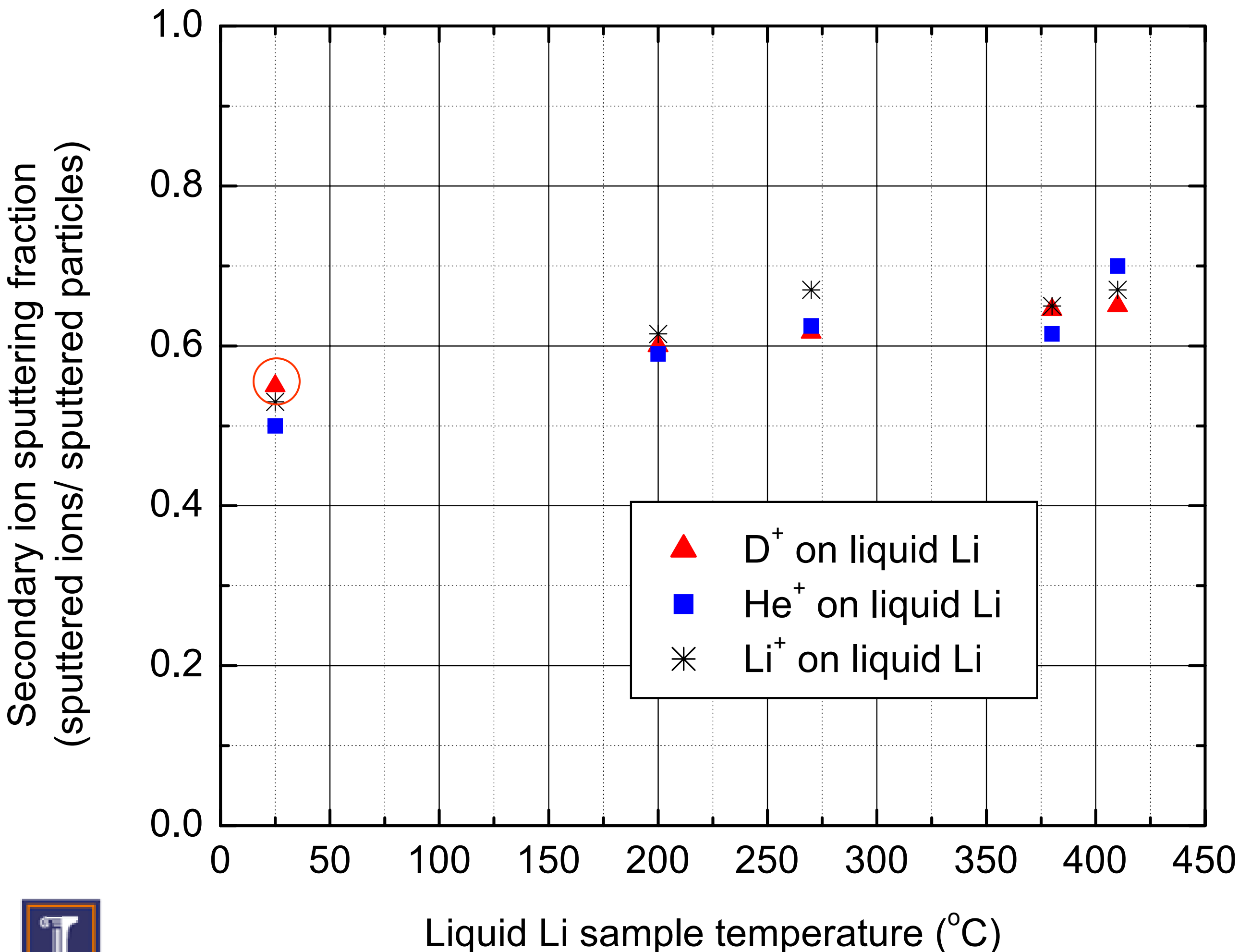
The ionization probability is then obtained after two fitting parameters, α and Δ_o are fitted to experimental data. Then one sums over *n* trajectories to obtain an average probability[1].

$$P^{+} = \exp\left[\frac{-2\Delta(z_c)}{\hbar\alpha v_p}\right]$$

$$P^{+}_{total} \equiv \sum_{N=1}^{n} \frac{P^{+}_{N}(v_p,\Omega)}{N}$$

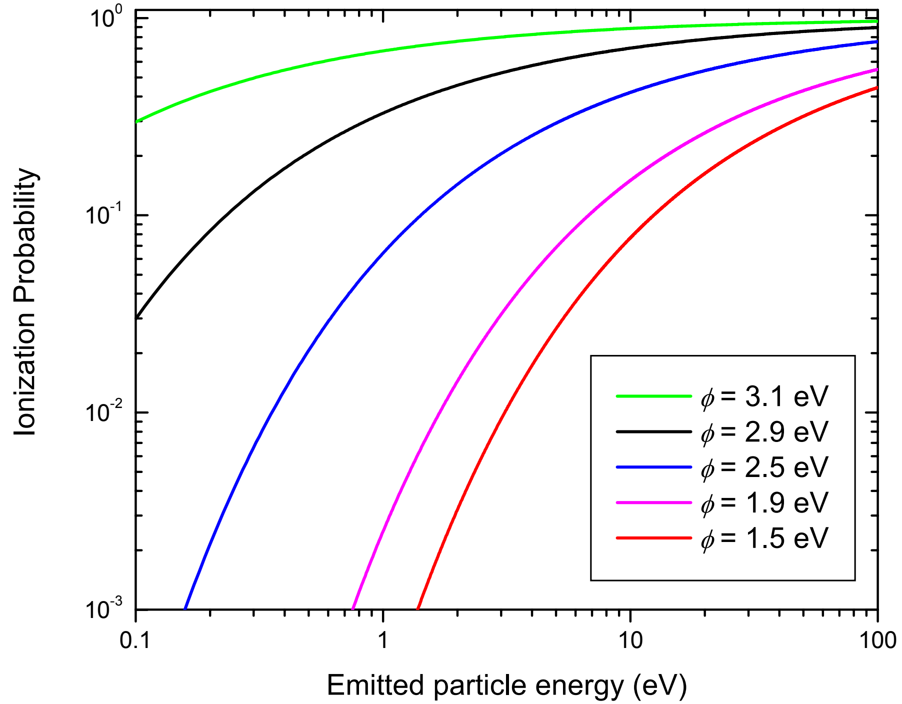
1. G.A. Kimmel, et al. Phys. Rev B 43 (12) (1991) 9403.

Secondary ion sputtering fraction (Y^{+}_{sp}) dependence on target temperature for Liquid Lithium

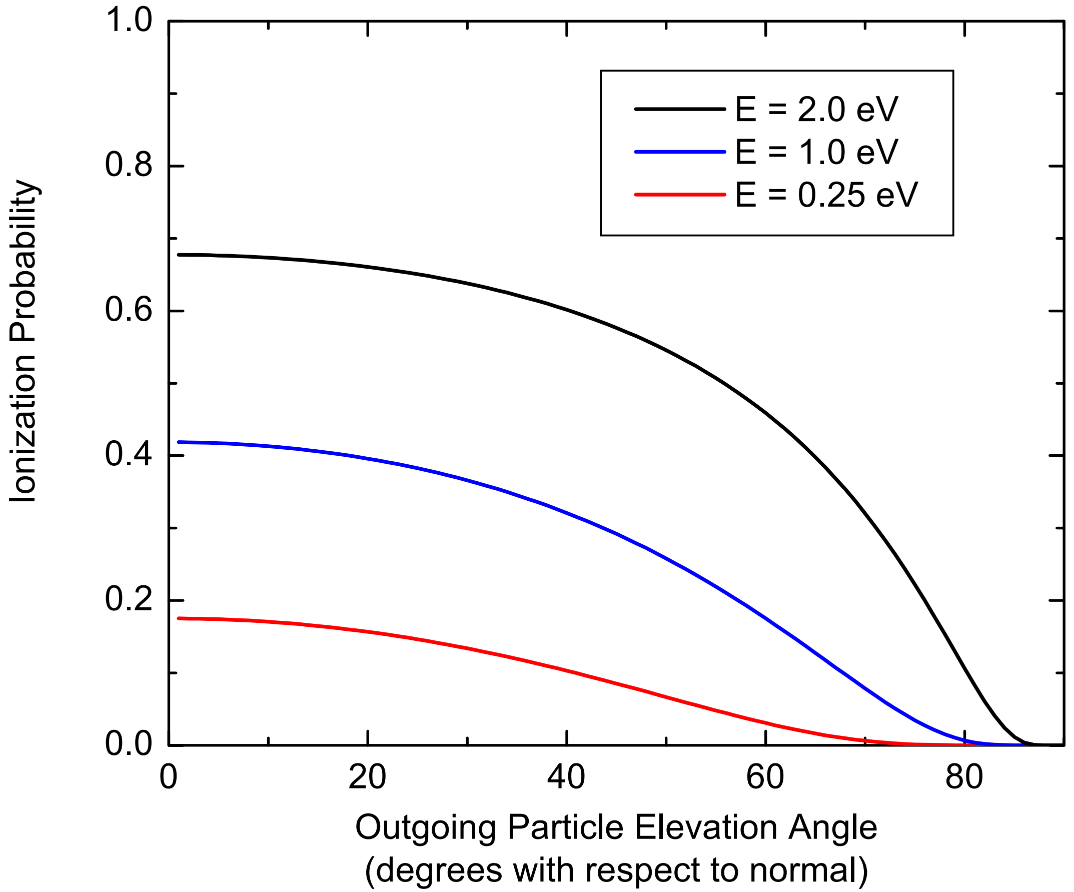


Andersen-Newns Model

Ionization probability of backscattered alkali atoms at low energy



- The ionization probability has a strong dependence on outgoing velocity and surface work function (which depends on the surface thermodynamic and chemical state).
- At lower outgoing velocities and oblique emissions, alkali backscattered atoms are neutralized near the surface.

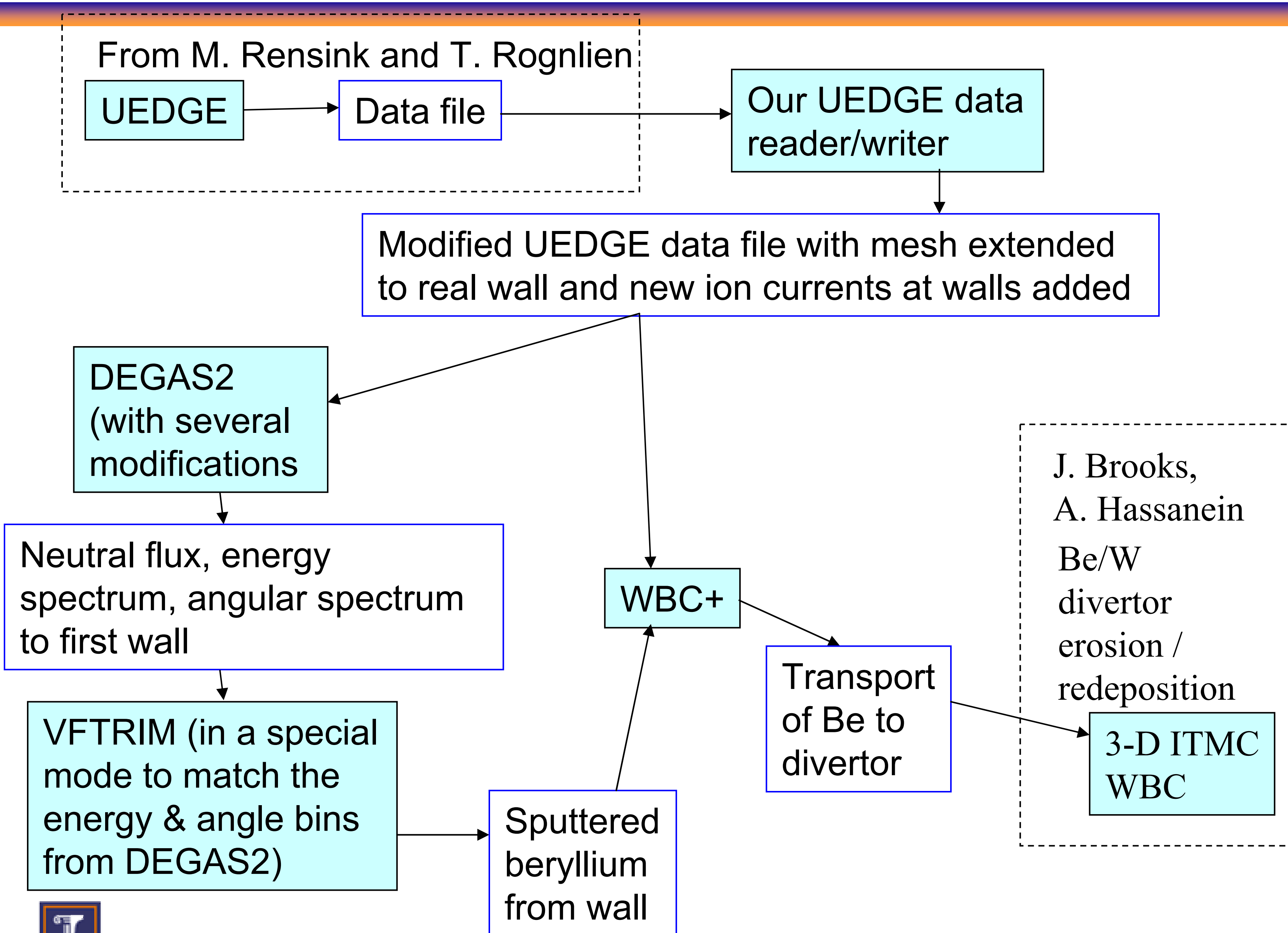


- For liquid lithium without any adsorbates or oxides the average surface work function is 2.9 eV[1]. For the case of 0.35 eV incident Li^+ at 20-degree incidence, the average backscattered energy is 0.25 eV with an average elevation angle of 15 degrees. Its ion probability is about 20%

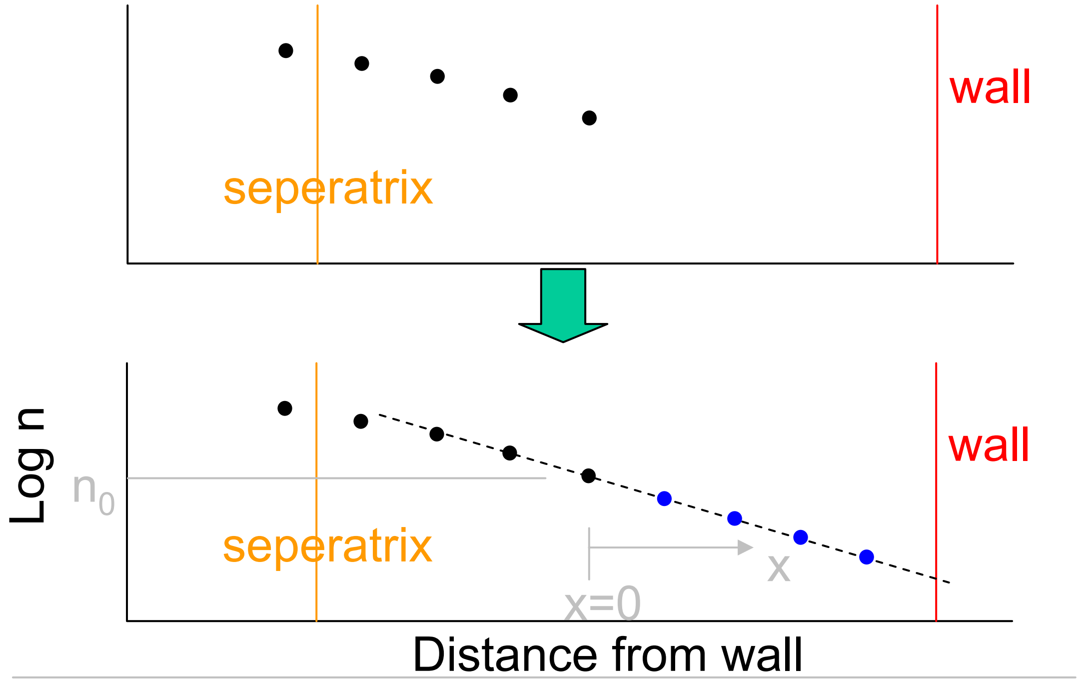
1. N.W. Aschcroft and N.D. Mermin, Solid State Physics, 1976, Saunders College Publishing

NSO/FIRE Modeling

- Current focus - beryllium/tungsten mixed material erosion issues
- Beryllium from first wall is sputtered, and transported to the divertor
- Result is a Be/W mixture on the divertor surface
- Erosion behavior of this mixed material is critical to FIRE divertor performance
- Collaborative modeling effort, combining several computer codes
  - UEDGE, DEGAS2, VFTRIM, WBC, ITMC


From M. Rensink and T. Rognlien
UEDGE
Data file
Our UEDGE data reader/writer
Modified UEDGE data file with mesh extended to real wall and new ion currents at walls added
DEGAS2 (with several modifications
Neutral flux, energy spectrum, angular spectrum to first wall
VFTRIM (in a special mode to match the energy & angle bins from DEGAS2)
Sputtered beryllium from wall
WBC+
Transport of Be to divertor
J. Brooks, A. Hassanein
Be/W divertor erosion / redeposition
3-D ITMC WBC

Extrapolation of plasma parameters from UEDGE out to real wall

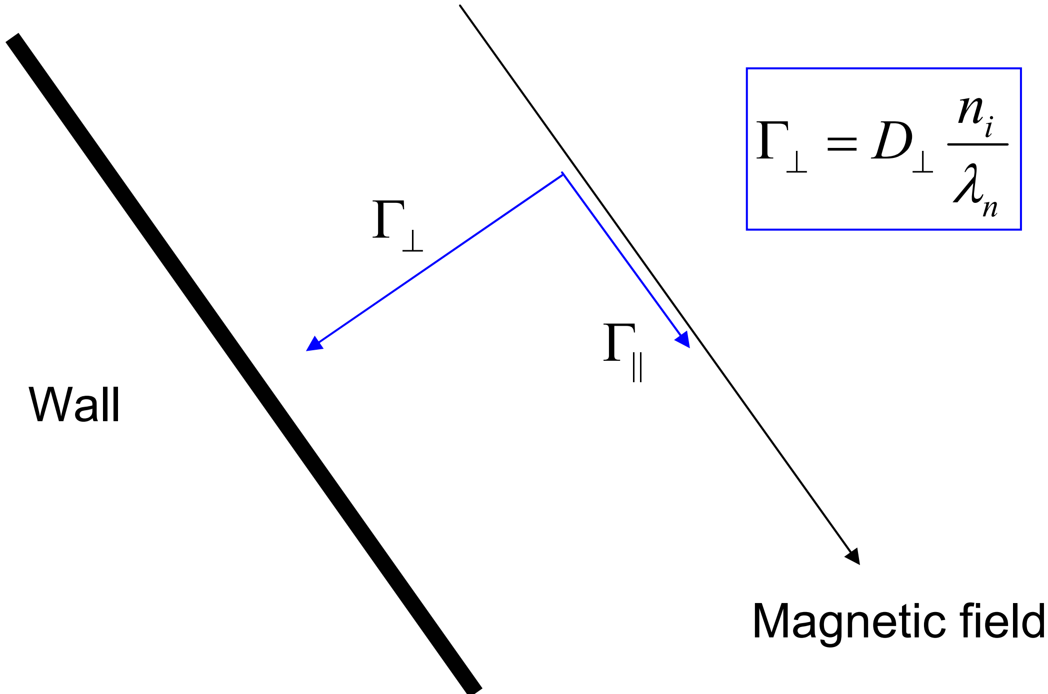


Plasma parameters are calculated from some scrape-off length, as in

$$n(x) = n_0 \exp\left(\frac{-x}{\lambda_i}\right)$$

where λ_i is calculated to fit the outermost zones in each i row.

Model for ion flux to wall



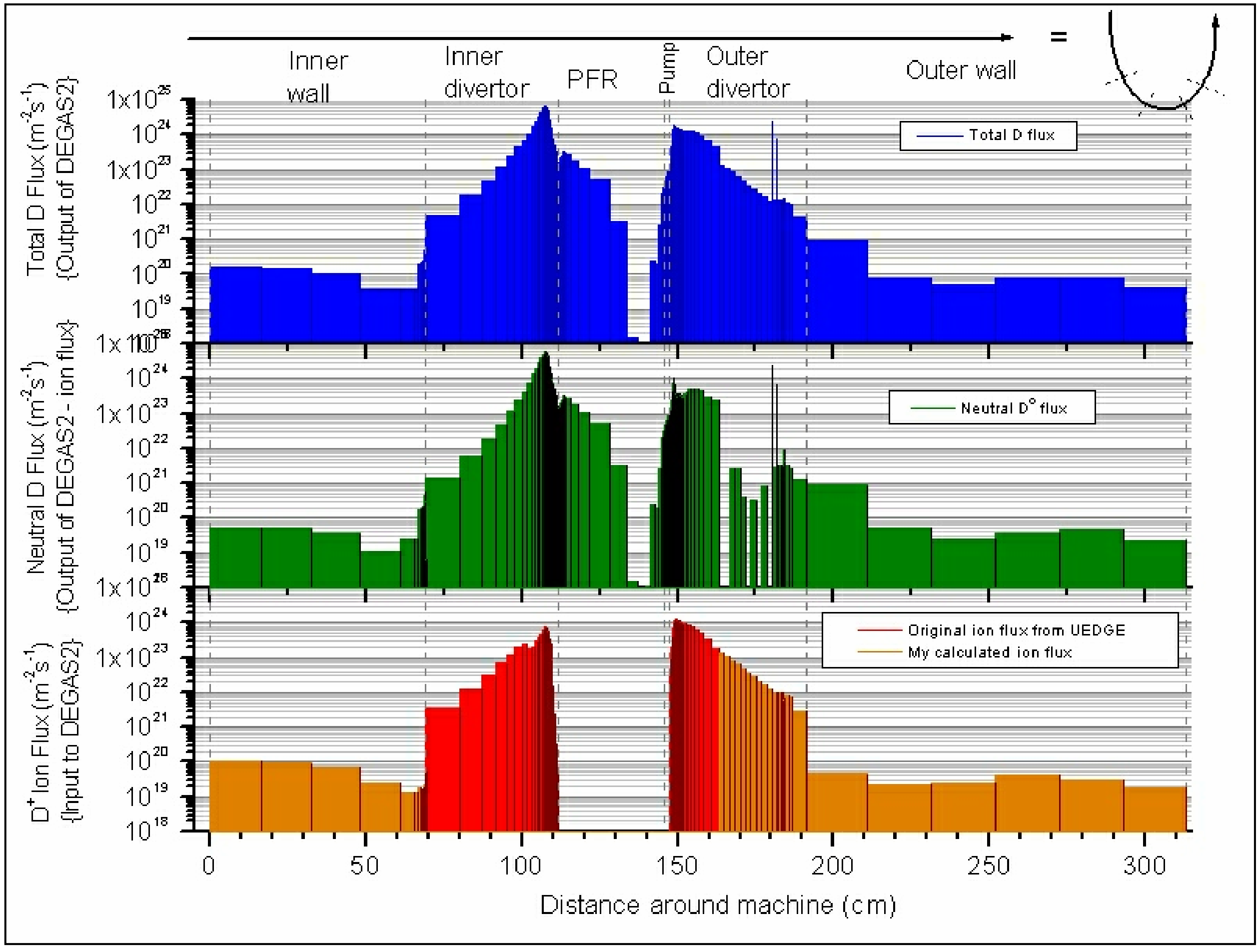
$$\Gamma_\perp = D_\perp \frac{n_i}{\lambda_n}$$

$$D_{Bohm} \cong 0.06 \frac{T_e}{B}$$

- Since the wall is tangent to the magnetic field, the flux comes from cross-field diffusion
- The perpendicular diffusion coefficient is estimated as the Bohm diffusion coefficient
- Anomalous cross-field transport model is now included and simulations are underway

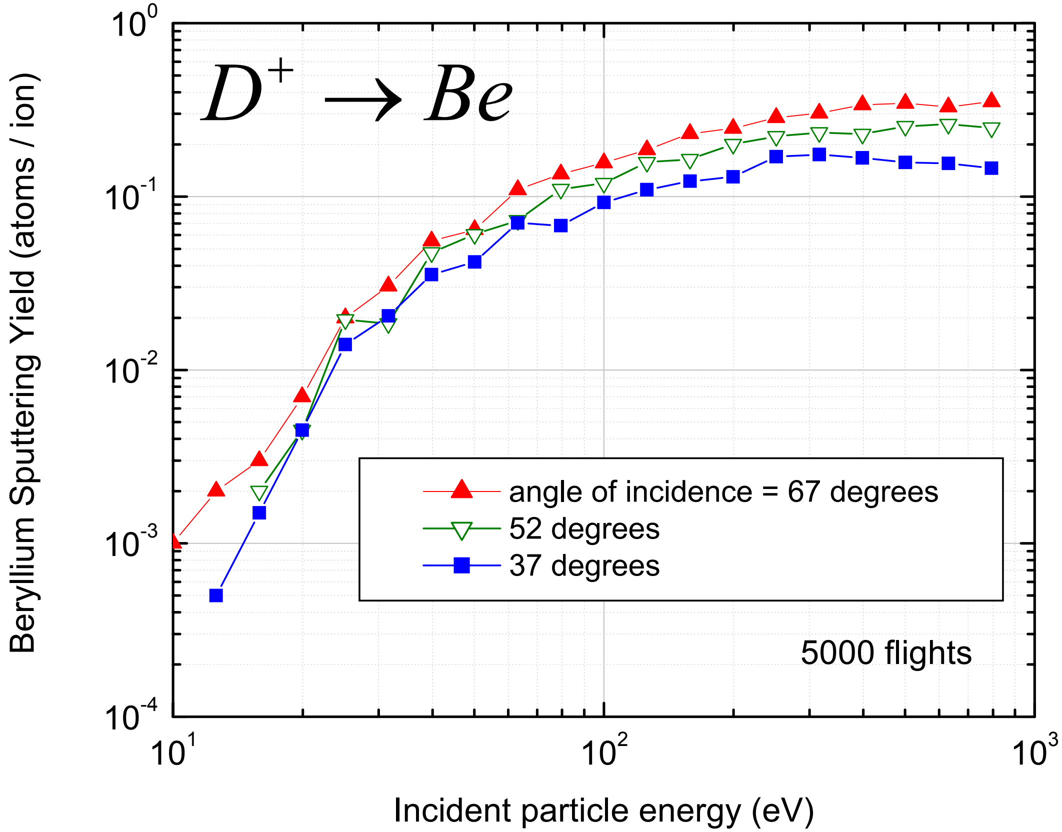
FIRE Be/W mixed material analysis

- Included fueling sources in DEGAS2 modeling
  - 100 torr/l-s pellet injection
  - 100 torr/l-s gas puffing
- Be sputtering source from first wall is 8.9×10^{19} s^{-1}
- WBC+ analysis shows Be currents of
  - 4.1×10^{19} s^{-1} to inner divertor
  - 9.8×10^{18} s^{-1} to outer divertor



- Be net erosion to tungsten plates remains low – Anomalous diffusion model will lead to larger net erosion. Results will be presented at APS-DPP in Orlando, FL

VFTRIM-3D Modeling Results



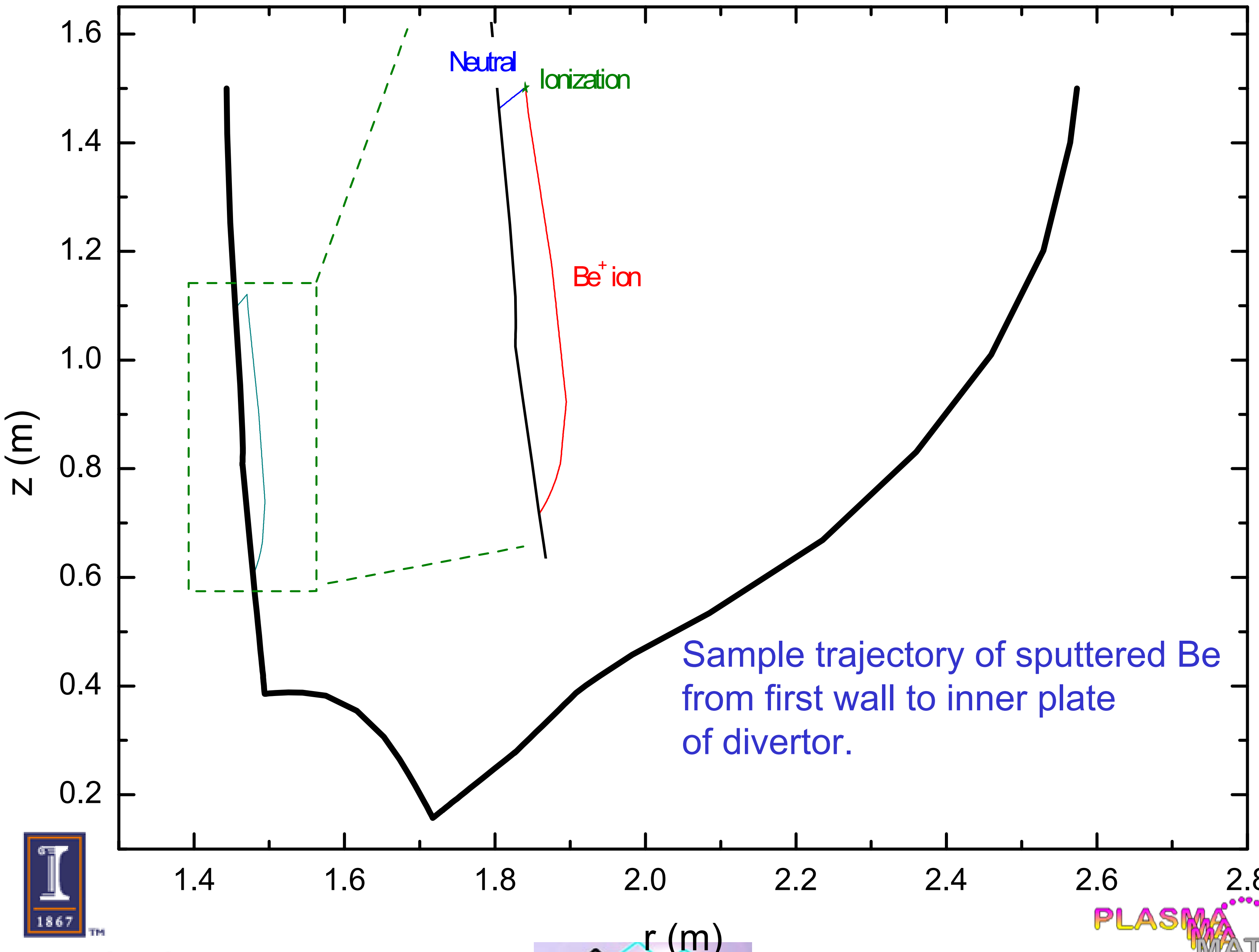
- Fractal dimension D = 2.05, Surface binding energy = 3.38 eV.
- Binary collision based on the Kr-C interaction potential and classical scattering kinematics.
- Electronic inelastic energy loss model uses an equipartition between the local Oen-Robinson model and non-local Lindhard-Sharff model.

ILLINOIS

PLASMA MATERIAL INTERACTION GROUP
University of Illinois at Urbana-Champaign

Summary of WBC+ code

- Impurity transport code obtained from J.N. Brooks
- Determines the flux of Be from the wall arriving on the divertor
- Inputs to WBC+
  - FIRE Geometry & plasma background from modified UEDGE data
  - Results of DEGAS2/VFTRIM calculations
    - Flux of sputtered Be from the walls
    - Energy & angular distributions of sputtered Be
- Method
  - Particles are launched randomly by sampling the Be sputtering distributions obtained from VFTRIM
  - Neutrals move in straight line until ionized
  - Once ionized, they follow the magnetic field lines
  - Particles tracked until they hit a surface

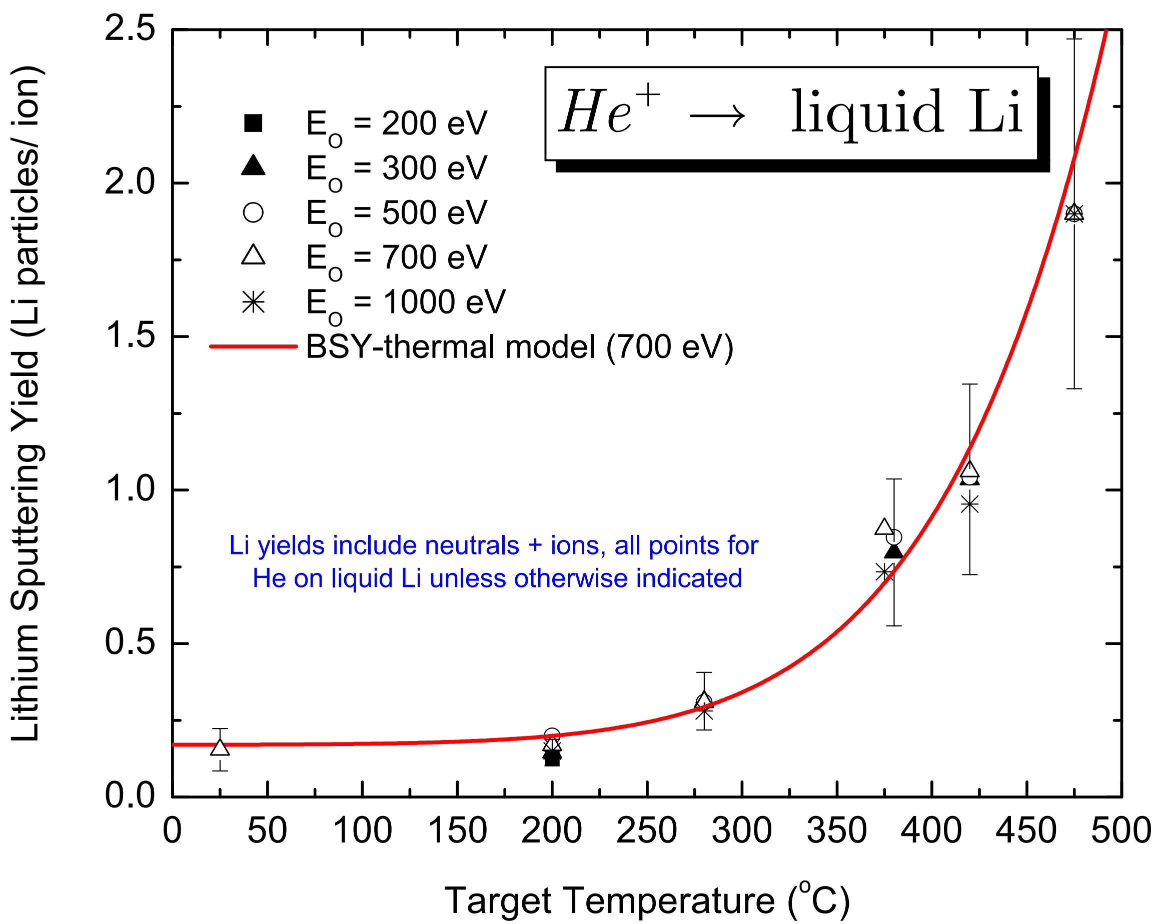


Sample trajectory of sputtered Be from first wall to inner plate of divertor.

ILLINOIS

PLASMA MATERIAL INTERACTION GROUP
University of Illinois at Urbana-Champaign

Liquid-metal erosion studies in IIAX



- Bohdansky-Sigmund-Yamamura thermal Model is shown to predict the temperature-dependent data of IIAX quite well for bombardment cases of He^+ on liquid lithium. Cases for D^+ and Li^+ bombardment are currently being investigated.

ILLINOIS 1867

Alps

PLASMA MATERIAL INTERACTION GROUP
University of Illinois at Urbana-Champaign

Temperature dependence modeling of liquid lithium

- Developing and understanding of lithium erosion enhancement by:
  - Molecular Dynamics simulations
  - Using semi-analytical models
- We are also utilizing VFTRIM-3D with modifications for the enhancement
  - NSTX modeling: temperature dependence of both total and differential sputtering yields

Future PMI Modeling Work Plan

- Continue study of hydrocarbon reflection from "soft" and "hard" graphite surfaces.
- Continued study of low energy liquid lithium reflection and sputtering under fusion-relevant conditions.
- Study of deuterium treatment on liquid lithium erosion and study of enhanced sputtering with molecular dynamics modeling of liquid lithium.
- FIRE runs on first wall/ divertor mixing problem.
- Continue modifications on VFTRIM-3D for both enhanced sputtering and capability of modeling dynamic composition changes on the target sample as well as local saturation effects